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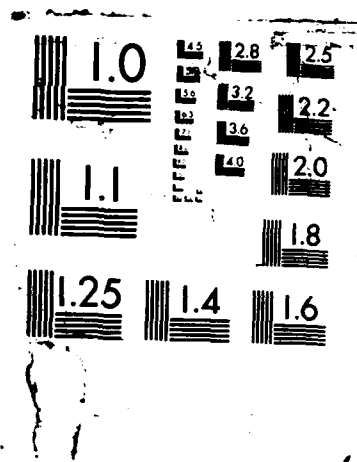   1987 AFOSR-TR-87-1724 AFOSR-84-0185 SEP 87

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The first and primary objective was to determine the correlation function describing large momentum pairing. A comparison of this correlation function with other correlations (such as singlet pairing, triplet pairing, charge density wave, and spin density wave) is now possible. The second objective was to strengthen and maintain a collaboration with researchers D.C. Reynolds and S.B. Nam at Wright-Patterson AFB. In light of the recent discovery of high temperature superconductivity (T(C) 95K) in rare earth copper oxide materials, it is apparent that a revolution in superconductivity research is beginning. This area will be of great importance to the Air Force in the future; thus close ties between University researchers and Air Force laboratories will be practical and beneficial.

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DR. ROBERT J. BARKER	(202)767-5011	NP

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LARGE MOMENTUM PAIRING IN
ONE-DIMENSIONAL SYSTEMS

Dr. D.W. Allender
Department of Physics and Liquid Crystal Institute
Kent State University
Kent, Ohio 44242

[Telephone: (216) 672-2577]

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I . Introduction and Statement of Accomplishments

This report summarizes the progress that was made on a theoretical investigation of large momentum pairing in one-dimensional superconductors that was proposed and supported by grant AFOSR-84-0185. The grant period from July 1984 to December 1985 was productive and successful in that two major objectives of the proposed research were achieved.

The first and primary objective was to determine the correlation function describing large momentum pairing. A comparison of this correlation function with other correlations (such as singlet pairing, triplet pairing, charge density wave, and spin density wave) is now possible. The second objective was to strengthen and maintain a collaboration with researchers D.C. Reynolds and S.B. Nam at Wright-Patterson AFB. In light of the recent discovery of high temperature super-conductivity ($T_C \sim 95K$) in rare earth copper oxide materials, it is apparent that a revolution in superconductivity research is beginning. This area will be of great importance to the Air Force in the future; thus close ties between University researchers and Air Force laboratories will be practical and beneficial.

In the remainder of this report, details are given about the first objective, and the facts regarding activities supported by this grant are presented.

II. The Large Momentum Pairing Correlation

In a review article in *Highly Conducting One-Dimensional Solids* (Plenum Press, NY, 1979), V.J. Emery presented a clear discussion of the theory of the one-dimensional electron gas. The model Hamiltonian he considered is often called the extended Hubbard model, and consists of three parts: (1) H_0 describing hopping from site to site, (2) H_1 giving on-site interaction, and (3) H_2 presenting intersite

interaction. H_1 and H_2 are mostly due to Coulomb effects, but phonons and other phenomena also contribute.

The standard correlation functions were described by Emery, and can be written as

$$\chi_\lambda^R = -i\theta(t)\left\langle\left[\hat{O}_\lambda^+(xt), \hat{O}_\lambda(00)\right]\right\rangle$$

where $\lambda = $ SP (singlet pairing), TP (triplet pairing), CDW (charge density wave), and SDW (spin density wave). The $\hat{O}_\lambda$ operators are

$$\hat{O}_{SP} = \psi_{2\sigma}^+\psi_{1-\sigma}^+$$

$$\hat{O}_{TP} = \psi_{2\sigma}^+\psi_{1\sigma}^+$$

$$\hat{O}_{CDW} = \frac{1}{\sqrt{2}}\left[\psi_{2\uparrow}^+\psi_{1\uparrow} + \psi_{2\downarrow}^+\psi_{1\downarrow}\right]$$

$$\hat{O}_{SDW} = \psi_{2\sigma}^+\psi_{1-\sigma}$$

The $\psi_{i\sigma}$ operators are the usual second-quantized fermion field operators. Label $i=1$ implies a particle with momentum to the right, label $i=2$ means momentum to the left, and σ denotes spin. The results found by evaluating these correlation functions using the full model Hamiltonian and the boson representation technique were

$$\chi_\lambda^R = \frac{\theta(t)}{2\pi^2 r^2} Im\left\{\left[r^2 K\left(x - v_s' t, r\right)K^*\left(x + v_s' t, r\right)\right]^{(\theta_s^{\pm 1}/2)}\right.$$

$$\times \left.\left[r^2 K\left(x - v_s' t, r\right)K\left(x + v_s' t, r\right)\right]^{(\theta_c^{\pm 1}/2)}\right\}.$$

The notation and functions in these equations are too cumbersome to carefully define in this report, but they are given by Emery. The important thing to notice is that the exponents $\theta_s^{\pm 1}$ and $\theta_c^{\pm 1}$ are functions of the parameters of the Hamiltonian.

The theoretical work carried out under this grant was a calculation of a new and previously unrecognized correlation function. Using the notation $\lambda = LMP$ (for large momentum pairing), and the definition

$$\hat{O}_{LMP} = \psi^+_{1\uparrow} \psi^+_{1\downarrow}$$

the correlation function χ^R_{LMP} was evaluated by means of the boson representation. The answer is

$$\chi_{LMP} = \frac{\theta(t)}{2\pi^2} \, Im \left\{ K^2\left(x - v'_c t, a\right) \left[r^2 K\left(x - v'_c t, r\right) K^*\left(x + v'_c t, r\right) \right]^{2\gamma} \right\}$$

where

$$2\gamma = -1 + \left(1 - \frac{\overline{W}_1^2}{4}\right)^{-1/2},$$

and all other notation is given by Emery ($\bar{W}_1$ is a parameter of the Hamiltonian).

The significance of this expression is that, by Fourier transforming, the exponent of the frequency dependence can be found. If the exponent is negative, the correlation diverges and one expects the ground state to have large momentum pairs formed. The Hamiltonian parameter values for which the exponent is negative can in principle be mapped out. These calculations to find the exponent have <u>not</u> been done, but are now possible. Further research effort to carry out these calculations is necessary.

III. Publications

The results of this research have not been published to date, although a manuscript is in preparation which presents the derivation of the results stated above in section II.

IV. Personnel

The research described here was pursued at Kent State University by the principal investigator, D.W. Allender. Two graduate students, Kazi Motakabbir and Young Hee Lee also carried out research and received support. Kazi received his Ph.D. in December 1985 and Young Hee completed his in August 1985.

V. Interactions

The primary interaction supported by this grant was the collaboration between D.C. Reynolds and S.B. Nam at Wright-Patterson AFB and the principal investigator. One trip was made to Wright-Patterson AFB where useful discussions were held.

Also supported was a presentation at the Midwest Solid State Theory Symposium in Minneapolis, MN in September 1984, as well as participation in two other conferences: the March 1985 meeting of the American Physical Society in Baltimore, MD and the Materials and Mechanisms of Superconductivity Conference in Ames, IA in May 1985.

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